The Summer Undergraduate Research Fellowship (SURF) Symposium
6 August 2015
Purdue University, West Lafayette, Indiana, USA

Molexpl: a tool for ab initio data exploration and visualization

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ABSTRACT

Density functional theory (DFT) based on ab initio theory, is a powerful method to resolve the electronic structure of atoms, molecules and solids. However, in practical, DFT is limited to few hundreds of atoms. To overcome this limitation, researchers have developed empirical interatomic potentials implemented in molecular dynamics (MD) simulations. MD ignores the movements of electrons and describes bonding and non-bonding interaction as a function of the distance between atoms called force fields (FF) or interatomic potentials. These empirical potentials are optimized against large datasets of DFT calculations relevant to describe the interactions between the atoms included in the training set. The Molexpl tool has been created to allow the user to explore a database of DFT calculations and to compare the results against classical MD simulations. The tool displays molecular structures and energy curves such as dissociation curve or equation of state. The initial database includes a set of elements that can be updated dynamically. The user can select multiple elements, and can choose between running MD or explore the database of DFT calculations. Moreover, Molexpl allows the user to upload a force-field (FF) or a training set for more specific research purpose. Finally, this tool can serve as a portal to share fundamental properties of molecules and crystals with the scientific community or be used as a data visualizer in the classroom. Beyond the academic purpose, this tool can help to judge the quality of a FF applied to a specific problem.

KEYWORDS

density functional theory, ab initio, molecular dynamics, molecular exploration